Chemistry and kinematics of the pre-stellar core L1544: Constraints from H_2D^+.

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This paper explores the sensitivity of line profiles of H_2D^+, HCO^+ and N_2H^+, observed towards the center of L 1544, to various kinematic and chemical parameters. The total width of the H_2D^+ line can be matched by a static model and by models invoking ambipolar diffusion and gravitational collapse. The derived turbulent line width is b=0.15 km s^{-1} for the static case and $\lesssim$0.05 km s^{-1} for the collapse case. However, line profiles of $HC^{18}O^+$ and N_2H^+ rule out the static solution. The double-peaked H_2D^+ line shape requires either infall speeds in the center that are much higher than predicted by ambipolar diffusion models, or a shell-type distribution of H_2D^+, as is the case for HCO^+ and N_2H^+. At an offset of $\approx 20''$ from the dust peak, the H_2D^+ abundance drops by a factor of $\approx$5.

1 Introduction

Deuterium-bearing molecules are important as probes of the very cold phases of molecular clouds prior to star formation. The H_2D^+ ion is especially important as tracer of H_3^+, the primary ion in dense molecular clouds, which does not have a dipole moment and hence no pure rotational lines. In addition, at low temperatures ($\lesssim$10 K), H_2D^+ has the ability to channel D atoms from their main reservoir, HD, into heavier species. This process leads to abundance ratios of DCO^+/HCO^+ and N_2D^+/N_2H^+ of $\sim 10^{-3} - 10^{-1}$ observed towards dense cores, much larger than the elemental D/H ratio of $\sim 10^{-5}$. Recent observations of multiply deuterated H_2CO, CH_3OH, H_2S and NH_3 (see Ceccarelli, this volume) suggest that under extreme conditions, a significant fraction of D may be transferred to heavy molecules. We wish to quantify the role of H_2D^+ in this process, and compare with other processes such as grain surface reactions (Caselli, this volume).

The ground-state 1_{01}–0_{00} transition of para-H_2D^+ at 1370 GHz will be a prime target for GREAT on SOFIA. However, with the upper energy level

65 K above ground, this line will only be excited in relatively warm ($\gtrsim 20$ K) regions, where chemical fractionation is ineffective. For colder sources, the 1_{10}–1_{11} ground-state transition of ortho-H_2D^+ at 372 GHz is more suitable, which can be observed from the ground under good conditions. At the low temperatures ($\lesssim 10$ K) and high densities ($> 10^5$ cm^{-3}) of pre-stellar cores, reactive collisions with ortho–H_2 keep the ortho-para ratio of H_2D^+ at $\sim$1, orders of magnitude above the LTE value [1, 2].

Until 2002, only two detections of H_2D^+ had been obtained, which indicated abundances of $\sim 10^{-11}$–10^{-12} towards Class 0 objects [3, 4]. In October 2002, we [5] observed strong H_2D^+ emission towards the pre-stellar core L 1544, and derived an abundance of $\sim 1\times10^{-9}$ in the central $\approx 20''$. Such a high abundance suggests that in this region, all CNO-bearing species are depleted onto dust grains, a situation explored in more detail by Walmsley (this volume). Data taken in June 2003 at the CSO indicate that the same phenomenon takes place in at least five other pre-stellar cores. More observations are scheduled for December 2003. These data will be presented in a forthcoming paper. Here we investigate the line profile of H_2D^+ in L 1544, and derive its abundance outside the central region.

2 Kinematics

The line profile of H_2D^+ towards L 1544 appears double-peaked, although the signal-to-noise ratio is not high (Fig. 1). Fitting two Gaussians to the profile yields results very similar to those for the profiles of $HC^{18}O^+$, $D^{13}CO^+$ and N_2H^+, observed by [6]: two thermal components separated by $\approx$0.26 km s^{-1} (Table 1). We therefore investigate whether the kinematic models that fit the HCO^+ and N_2H^+ data also reproduce the H_2D^+ line profile.

Table 1. Centroids and widths of the two velocity components. Numbers in brackets denote uncertainties in units of the last decimal.

Line	$V_{\rm LSR}$ km s^{-1}	$\Delta V_{\rm obs}$ km s^{-1}	$\Delta V_{\rm T}^a$ km s^{-1}
H_2D^+ (1_{10}–1_{11})	7.06(3)	0.22(5)	0.28–0.34
	7.34(2)	0.25(6)	
$HC^{18}O^+$ (1–0)	7.04(1)	0.18(3)	0.10–0.12
	7.28(1)	0.23(3)	
$D^{13}CO^+$ (2–1)	7.08(2)	0.20(4)	0.10–0.12
	7.35(4)	0.20(8)	
N_2H^+ (1–0, F_1F=10–11)	7.08(1)	0.19(1)	0.11–0.13
	7.33(1)	0.20(2)	

[a] Thermal line width at $T_{\rm kin}$=7 and 10 K.

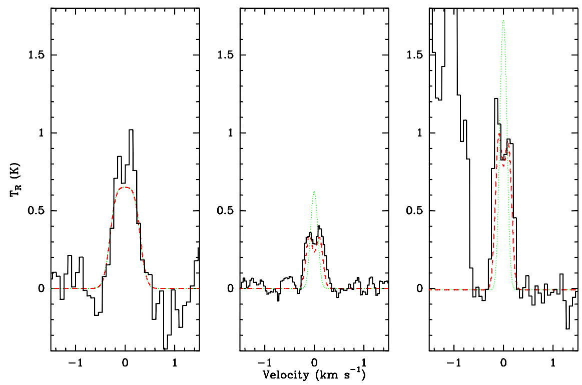

Fig. 1. Observed line profiles of H_2D^+ (left), $HC^{18}O^+$ (middle) and N_2H^+ (right), and synthetic profiles for the static (dotted) and infall (dashed) models.

The line profile of H_2D^+ was modeled using a Monte Carlo radiative transfer program [7] [5]. Figure 2 shows the adopted temperature and density structure of L1544, taken from [8]. See [5] for details of the excitation model; at $T_{\rm kin} \lesssim 10$ K, ortho-H_2D^+ is essentially a two-level system, so that our results are not sensitive to the collision rates of non-radiative transitions between high-lying levels. For H_2D^+ we adopt an abundance of 1×10^{-9} in the central 20″ [5]. For HCO^+, DCO^+, N_2H^+ and N_2D^+, we used the abundance profiles from [9], Model 3, and assumed zero abundance inside r=2500 AU. We explored static models, and models with velocity fields from the ambipolar diffusion models 't3' and 't5' of [10] (see [6] for details). For the turbulent broadening, Doppler parameters b between 0.05 and 0.25 km s^{-1} were tried. Smaller values of b are overwhelmed by thermal broadening; larger ones do not fit the data.

We find that the total width of the H_2D^+ line can be matched using either velocity field. While the best-fit static model has b=0.15, b=0.05 gives the best fits with the infall velocity fields. However, the $HC^{18}O^+$ and N_2H^+ J=1-0 observations from [6] rule out the static model, which does not give a double-peaked line shape. Using the infall velocity fields, the data are matched with b=0.05, consistent with the H_2D^+ results (Fig. 1).

None of our adopted velocity fields reproduces the double-peaked H_2D^+ line shape that the observations indicate. One possibility is that the infall speeds of ≈0.1 km s^{-1} continue further inwards than in the models by [10]. Alternatively, the distribution of H_2D^+ may have a central hole, not because of adsorption onto dust grains (as for CO and N_2, the precursors of HCO^+ and N_2H^+), but due to conversion into D_2H^+ and D_3^+.

[5] http://www.mpifr-bonn.mpg.de/staff/fvandertak/ratran/

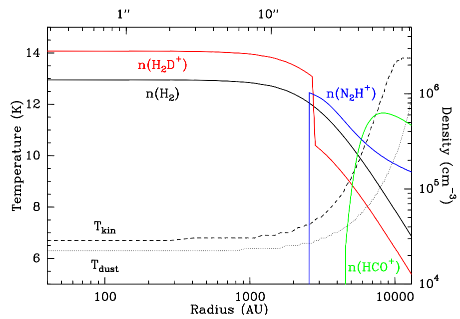

Fig. 2. Radial profiles of dust and gas temperature, and the densities of H_2, H_2D^+ ($\times 2\times 10^9$), HCO^+ ($\times 10^{12}$) and N_2H^+ ($\times 10^{10}$) in our model of L 1544.

3 Abundance profile of H_2D^+

The abundance of H_2D^+ away from the dust peak of L 1544 was estimated to be a factor of two lower than toward the dust peak [5]. However, this abundance may be an overestimate because some fraction of the emission at the 20″ offset positions is pickup from the central core. We have run Monte Carlo models of the H_2D^+ emission, using the same temperature and density structure as before, and dropping the H_2D^+ abundance at a 20″ radius by factors of 2–10 from its central value of 1×10^{-9}. The H_2D^+ intensity at the 20″ offset position is best matched if the abundance drops by a factor of $\approx$5 at this radius. This result is independent of the velocity field. Models where this factor is 3 or 10 produce clearly worse matches to the data.

In a future paper, we will follow our results up with two-dimensional models and an exploration of different velocity fields. We will also model line profiles at offset positions.

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